

2-(propan-2-yl)-1,3,6-trioxocane
15351-38-9 | DTXSID80279934

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.76e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.84e-01

Confidence level: 7.21e-01

Nearest Neighbors from the Training Set

Image not found

Diethylene glycol diethyl ether

Measured: 6.16

Predicted: 3.11

Image not found

Butyl 3-methoxypropionate

Measured: 6.12e-02

Predicted: 6.04e-02

Image not found

propyl 3-methoxypropanoate

Measured: 2.19e-01

Predicted: 2.08e-01

Image not found

Ethyl 3-ethoxypropionate

Measured: 3.80e-01

Predicted: 2.06e-01